

201-14300A

Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene)

CAS No. 10595-60-5

U. S. EPA HPV Challenge Program Submission

January 2003

Submitted by

Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195-1501

And
PPG Industries, Inc
One PPG Place
Pittsburgh, PA 15272

RECEIVED
OPPT/MCIC
2003 FEB 14 PM 2:53

TEST PLAN

Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene)
CAS No. 10595-60-5

HPV End Point	Information Available (Yes/No)	Acceptable (Yes/No)	Surrogate Data (Yes/No)	Testing Required (Yes/No)
Physical-chemical Data				
Melting Point	No			No
Boiling Point	No			No
Vapor Pressure	Yes	Yes		No
Water Solubility	No		Yes	No
Partition Coefficient	Yes	Yes		No
Environmental Fate and Pathway				
Photodegradation	Yes	Yes		No
Stability in Water	Yes	Yes		No
Transport/distribution (Fugacity)	Yes	Yes		No
Biodegradation	No		Yes	No
Ecotoxicity				
Acute toxicity to fish	No		Yes	No
Acute toxicity to <i>daphnia</i>	No		Yes	No
Acute toxicity to algae	No		Yes	No
Toxicity				
Acute Toxicity	Yes	Yes		No
Repeated Dose Toxicity	No		Yes	No
Toxicity to Reproduction/Developmental toxicity	No		Yes	No
Genetic toxicity <i>in vitro</i> (Gene Mutation)	No		Yes	No
Genetic toxicity <i>in vitro</i> (Chromosomal Aberration)	No		Yes	No

TABLE OF CONTENTS

1.	Sponsoring Companies	4
2.	Test Substance	4
3.	Criteria for Determining Adequacy of Data.....	4
4.	Test Plan	5
4.1	Physical/Chemical Properties	5
4.2	Environmental Fate/Pathways.....	5
4.3	Ecotoxicity	6
4.4	Human Health Data.....	7
4.4.1	Acute Mammalian Toxicity	7
4.4.2	Repeated Dose Mammalian Toxicity.....	7
4.4.3	Genetic Toxicity.....	7
4.4.4	Reproductive/Developmental Toxicity	7
5.	Summary	7
6.	References.....	8
7.	Appendix 1-Robust Summaries	

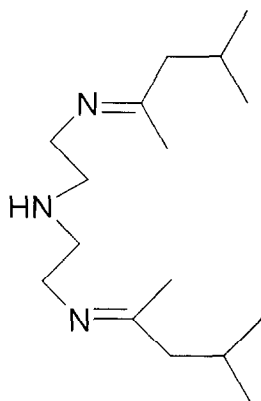
1. Sponsoring Companies

Air Products and Chemicals, Inc. and PPG Industries, Inc. are the manufacturers of Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) and are the joint sponsors of this substance for the U.S. Environmental Protection Agency's HPV Chemical Challenge Program. The technical contact is

Dr. James Barter
PPG Industries, Inc.
One PPG Place
Pittsburgh, Pennsylvania 15272
Phone (412) 434-2801

2. Test substance

Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) is a single chemical substance. The major use is for the production of paint products. Its molecular structure is as follows:



The test substance is produced in the presence of excess Methyl Isobutyl Ketone (MIBK) (~30%). At this concentration, the material is a clear, light yellow, very fluid liquid. An attempt was made to drive off the MIBK by distillation when the test substance was prepared for HPV testing. However, this attempted removal of the excess MIBK solvent from the substance resulted in formation of polymeric by-products. Therefore, the production batch (70% test substance in 30% MIBK) was used for testing.

3. Criteria for Determining Adequacy of Data

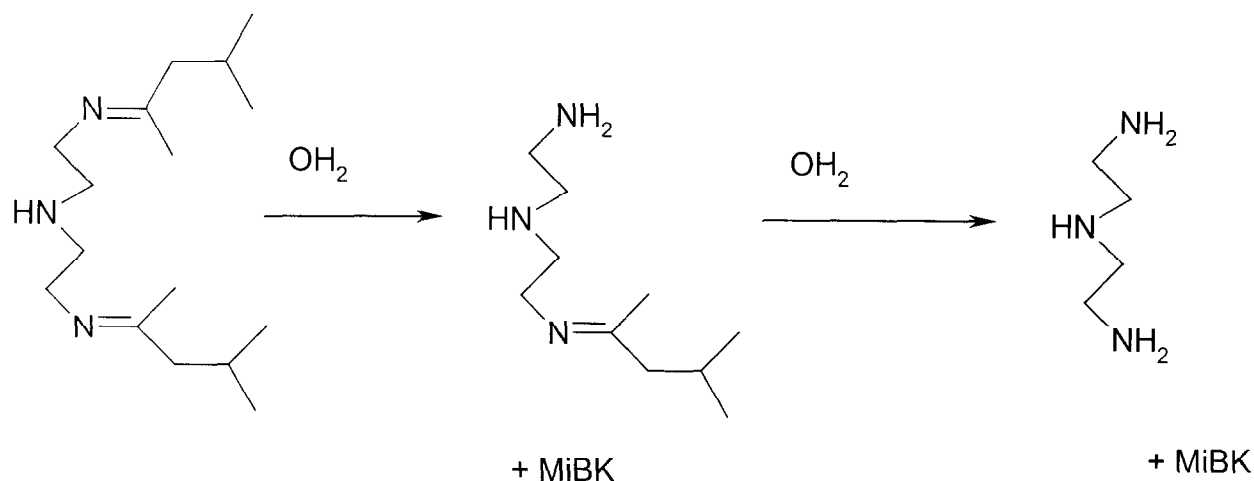
All relevant studies were reviewed and assessed for adequacy according to the standards of Klimisch *et al.* (1977). Four reliability categories, 1-reliable without restriction, 2-reliable with restriction, 3-not reliable, and 4-not assignable, have been established and a rating of 1 and 2 were considered to be adequate.

4. Test Plan

4.1 Physical/Chemical Properties

No data are available for melting point, boiling point, and water solubility. Because producing pure material (free of MIBK) for the purposes of determining a melting point and a boiling point is not possible, no meaningful data for melting and boiling points can be generated. In addition, the substance will probably begin to decompose before it boils, especially at atmospheric pressure. Therefore, no testing for these endpoints is recommended.

The test substance, Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) is rapidly hydrolyzed to Diethylenetriamine (DETA) and MIBK within minutes (*see section below for the details*).



If the quantity of the test substance added to water is high enough, the MIBK that is produced will exceed its solubility (1.9%) in water and a separate phase of MIBK will result. Due to the rapid hydrolysis, the water solubility of this material is expected to be limited to the solubility of DETA. Therefore, the water solubility of the test substance should be referenced to the DETA data. Both MIBK and DETA are listed under the EPA HPV Challenge Program and these chemicals are being handled under the Organization for Economic Cooperation and Development (OECD) HPV Screening Information Data Set (SIDS) Program. Data for vapor pressure and partition coefficient (K_{ow}) are estimated (calculated) using a modeled approach. No testing is recommended.

4.2 Environmental Fate/Pathways

Results of the two hydrolysis studies indicate that the test substance is rapidly hydrolyzed to DETA (CAS number 111-40-0) and MIBK (CAS number 108-10-1). The calculated half-life in the first study (Springborn report, 2002) ranges from 1.31 minutes to 34.5 minutes depending on the pH of the test solutions.

Hydrolytic rate constant and % Hydrolysis

<u>pH</u>	<u>Rate Constant (Kobs)</u>	<u>Calculate Half –Life (t_{1/2})</u>
1.2	1.44	28.9 minutes
4	1.21	34.5 minutes
7	11.5	3.61 minutes
9	0.53	1.31 minutes

In the second hydrolysis study (PPG Industries Analytical Report, 2002), greater than 90% of the test substance hydrolyzed within 5 minutes at all pH conditions.

Determination of Rate of Hydrolysis in different pH buffered conditions

<u>Time</u> (minutes)	<u>pH 1</u>	<u>pH 4</u>	<u>pH 7</u>	<u>pH 9</u>	<u>Distilled Water</u>
5	93.2%	94.5%	92.8%	87.9%	82.9%
15	94%	99%	98.9%	88.4%	90.8%
30	96.9%	99.7%	99.2%	92.7%	98.3%
60	98%	99.8%	100%	95.7%	100%

Since the test substance is produced in the presence of excess MIBK, which is used as a reflux solvent to assist in the removal of the product water via azeotropic distillation, only the presence of the one degradant DETA was confirmed in both studies.

Data for photodegradation and environmental transport are estimated using the EPIWIN/AOPWIN program. The estimated photodegradation hydroxyl radical rate constant is estimated to be $95.2679 \text{ E-12 cm}^3/\text{molecule-sec}$ with a half-life calculated to be 0.112 days. Level III fugacity modeling indicates that the test substance should partition to water (3.59%), air (0.078%), soil (27.3%), and sediment (69%). No data on biodegradability is available. However, due to the rapid hydrolysis of the test substance into DETA and MIBK in water, the biodegradability of DETA and MIBK can be referenced for this end point. No testing is recommended.

4.3 Ecotoxicity

This end point is filled from DETA and MIBK data. Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) is rapidly hydrolyzed (in minutes) to DETA and MIBK. Due to the rapid hydrolysis, the ecotoxicity of this material is expected to result from the hydrolysis products, DETA and MIBK. The ecotoxicity of this test substance should be referenced to the ecotoxicity data from DETA and MIBK. No testing is recommended.

4.4 Human Health Data

4.4.1 Acute Mammalian Toxicity

This endpoint is filled by one oral toxicity study in rats and one dermal toxicity study in rabbits (Carnegie Mellon Institute of Research Report, 1981). The oral LD₅₀ for Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) was 1.9 ml/kg and the dermal LD₅₀ value was >2.0 ml/kg. In addition, due to the rapid changes of the test substance into DETA and MIBK in acidic conditions, the acute oral toxicity data from DETA and MIBK can be referenced for this end point. The oral LD₅₀ of DETA and MIBK is reported as 1080 mg/kg and 2090 mg/kg, respectively in RTECS (Registry of Toxic Effects of Chemical Substances). No testing is recommended.

4.4.2 Repeated Dose Mammalian Toxicity

Due to the rapid hydrolysis of this test substance into DETA and MIBK under acidic conditions, the mammalian oral toxicity is expected to result from the hydrolysis products, DETA and MIBK. This end point should be referenced to the repeated dose mammalian toxicity study on DETA and MIBK. No testing is recommended.

4.4.3 Genetic Toxicity

Due to the rapid hydrolysis of this test substance into DETA and MIBK, the genetic toxicity is expected to result from the hydrolysis products, DETA and MIBK. Both MIBK and DETA are not considered to be mutagens in various genotoxicity studies (<http://cs3-hq.oecd.org/scripts/hpv/>). No testing is recommended.

4.4.4 Reproductive/Developmental Toxicity

Due to the rapid hydrolysis of the test substance into DETA and MIBK, the mammalian oral reproductive/developmental toxicity is expected to result from the hydrolysis products, DETA and MIBK. This endpoint should be referenced to reproductive/developmental toxicity on DETA and MIBK. No testing is recommended.

5. Summary

The test substance, Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene) rapidly hydrolyzes (within minutes) to DETA and MIBK. Several physical chemical properties and toxicity of this substance are expected to result from the hydrolysis products. Both MIBK and DETA are included in the EPA HPV Challenge Program and these chemicals are being handled under the Organization for Economic Cooperation and Development (OECD) HPV Screening Information Data Set (SIDS) Program. Therefore, data contained in the dossiers prepared for DETA and MIBK for the OECD SIDS program (<http://cs3-hq.oecd.org/scripts/hpv/>) should be utilized to fill data gaps for Diethylenetriamine, 1,7-bis(1,3-dimethylbutylidene).

6. References

- (1) Springborn Smithers Laboratories. Report 511.6215, Dated 10-29-02.
- (2) PPG Industries Analytical Report No. CR10040, Dated 9-18-02.
- (3) Carnegie-Mellon Institute of Research report No. 81-21S, Dated 3-13-81.